Variational Methods for Latent Variable Problems (part 2)

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Outline for today:

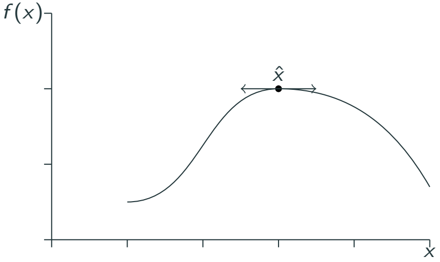
- What counts as variational inference?
- Kullback-Leibler (KL) divergence and “standard” variational inference
- The classical EM algorithm as a special case of variational inference
- Variational inference as a generalization of the EM algorithm
- A quick and incomplete sketch of further topics in variational inference

What counts as variational inference?

Lots of very different procedures go by the name "variational inference." I propose an (idosyncratic) enompassing definition based on the use cases and the name:

Variational inference is inference using optimization.

Think "calculus of variations:" an optimum $\hat{x} = \underset{\theta}{\operatorname{argmax}} f(x)$ is characterized by $df/dx|_{\hat{x}} = 0$, i.e. where small variations in $\hat{x}$ result in no changes to the value of $f(\hat{x})$.



By this definition,

- The maximum likelihood estimator (MLE) is VI.
- The Laplace approximation to a Bayesian posterior is VI.
- Markov chain Monte Carlo (MCMC) is not VI.

What counts as variational inference?

A more common definition of VI is the following.

Suppose we have a random variable ξ and a distribution $\mathfrak{p}(\xi)$ that we want to know.

Let y denote data and θ a parameter. Examples:

- The variable is θ, and we wish to know the posterior $\mathfrak{p}(\theta|y)$ (Bayes)
- The variable is y, and we wish to know $\mathfrak{p}(y)$ (MLE)
- The variable is y, and we wish to know the map $\theta \mapsto \mathfrak{p}(y|\theta) = \int p(y, z|\theta)dz$ (marginal MLE)

Let $\mathcal{Q}$ be some class of distributions which may or may not contain $\mathfrak{p}(\xi)$.

Variational inference finds the distribution in $\mathcal{Q}$ closest to $\mathfrak{p}$ according to some measure of "divergence" between distributions:

$$\mathfrak{q}^* = \operatorname*{argmin}_{\mathfrak{q} \in \mathcal{Q}} D(\mathfrak{q}, \mathfrak{p}).$$

The most common choice of "divergence" is the **Kullback-Leibler** (KL) divergence, though other choices are possible (e.g. Li and Turner [2016], Liu and Wang [2016], Ambrogioni et al. [2018]).

KL divergence

The KL divergence is defined as:

$$\mathrm{KL}\left(\mathfrak{q}||\mathfrak{p}\right) := \underset{\mathfrak{q}(\xi)}{\mathbb{E}}\left[\log \mathfrak{q}(\xi)\right] - \underset{\mathfrak{q}(\xi)}{\mathbb{E}}\left[\log \mathfrak{p}(\xi)\right]$$

Some points to be aware of:

- $\mathrm{KL}\left(\mathfrak{q}||\mathfrak{p}\right) \geq 0$
- $\mathrm{KL}\left(\mathfrak{q}||\mathfrak{p}\right) = 0 \Rightarrow \mathfrak{p} = \mathfrak{q}$
- $\mathrm{KL}\left(\mathfrak{q}||\mathfrak{p}\right) \neq \mathrm{KL}\left(\mathfrak{p}||\mathfrak{q}\right)$
- $\mathrm{KL}\left(\mathfrak{q}||\mathfrak{p}\right)$ is a "strict" measure of closeness [Gibbs and Su, 2002]

Why use KL divergence?

Phony answer: The KL divergence has an information theoretic interpretation [Kullback and Leibler, 1951].

Real answer: Mathematical convenience (normalizing constants pop out).

Example: the MLE minimizes KL divergence. Suppose that $x_n \overset{iid}{\sim} \mathfrak{p}(\cdot)$, and $\mathfrak{q}(\cdot|\theta) \in \mathcal{Q}$ is a (possibly misspecified) parametric family of data distributions. Then

$$\begin{aligned}\hat{\theta} := \underset{\theta}{\mathrm{argmin}}\, \mathrm{KL}\left(\mathfrak{p}||\mathfrak{q}\right) = \underset{\theta}{\mathrm{argmin}} &\left(-\underset{\mathfrak{p}(x_1)}{\mathbb{E}}\left[\log \mathfrak{q}(x_1|\theta)\right] + \underset{\mathfrak{p}(x_1)}{\mathbb{E}}\left[\log \mathfrak{p}(x_1)\right]\right) \\ &= \underset{\theta}{\mathrm{argmax}}\, \underset{\mathfrak{p}(x_1)}{\mathbb{E}}\left[\log \mathfrak{q}(x_1|\theta)\right] \approx \underset{\theta}{\mathrm{argmax}}\, \frac{1}{N}\sum_{n=1}^{N} \log \mathfrak{q}(x_n|\theta).\end{aligned}$$

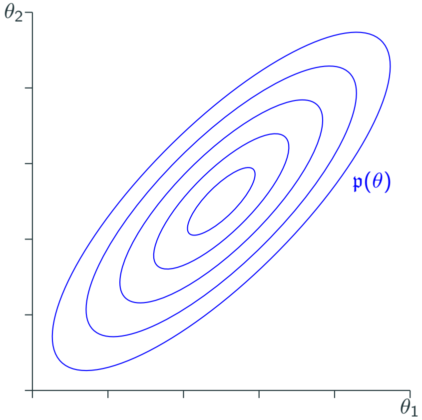
KL divergence exercises

$$\mathrm{KL}\left(\mathfrak{q}(\theta)||\mathfrak{p}(\theta)\right) = \\ -\mathop{\mathbb{E}}_{\mathfrak{q}(\theta)}[\log \mathfrak{p}(\theta)] + \mathop{\mathbb{E}}_{\mathfrak{q}(\theta)}[\log \mathfrak{q}(\theta)]$$

$$\mathfrak{p}(\theta) = \text{Correlated bivariate normal}$$

$$\mathcal{Q} = \{\text{All bivariate normals}\}$$

What is $\mathfrak{q}^*(\theta) = \mathop{\mathrm{argmin}}_{\mathfrak{q} \in \mathcal{Q}} \mathrm{KL}\left(\mathfrak{q}(\theta)||\mathfrak{p}(\theta)\right)$?



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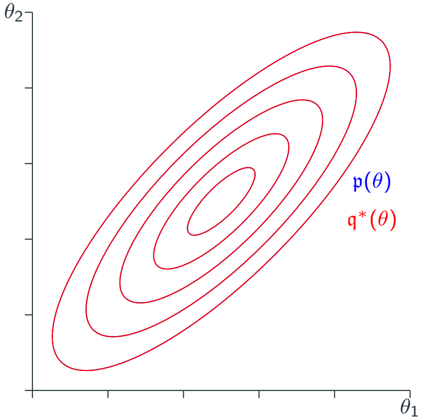

Sufficiently expressive families recover the target distribution.

KL divergence exercises

$$\mathrm{KL}\left(\mathfrak{q}(\theta)||\mathfrak{p}(\theta)\right) = - \underset{\mathfrak{q}(\theta)}{\mathbb{E}}\left[\log \mathfrak{p}(\theta)\right] + \underset{\mathfrak{q}(\theta)}{\mathbb{E}}\left[\log \mathfrak{q}(\theta)\right]$$

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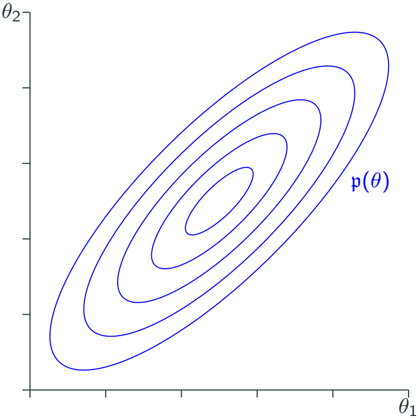

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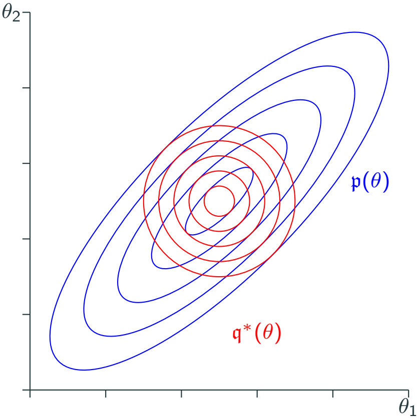

KL minimizers "fit inside" the second argument.

$$\mathrm{KL}\left(\mathfrak{p}(\theta) || \mathfrak{q}(\theta)\right) = \\ -\underset{\mathfrak{p}(\theta)}{\mathbb{E}}\left[\log \mathfrak{q}(\theta)\right] + \underset{\mathfrak{p}(\theta)}{\mathbb{E}}\left[\log \mathfrak{p}(\theta)\right]$$

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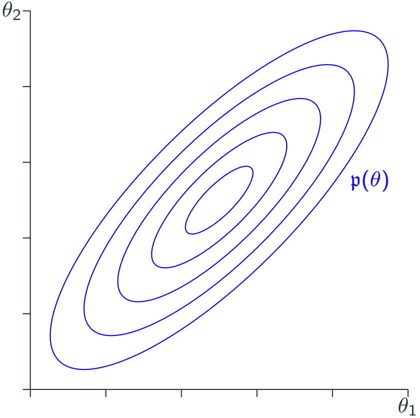

KL divergence exercises

$$\mathrm{KL}\left(\mathfrak{p}(\theta) || \mathfrak{q}(\theta)\right) =$$
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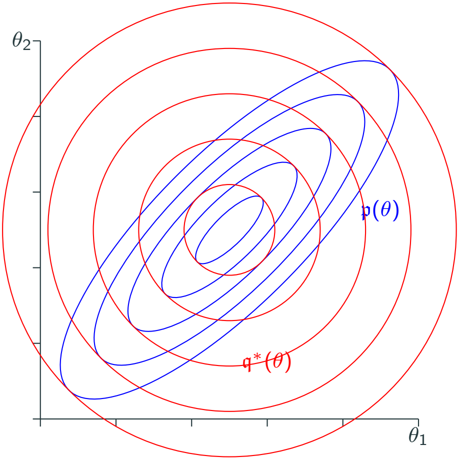

KL minimizers "fit inside" the second argument.

KL divergence exercises

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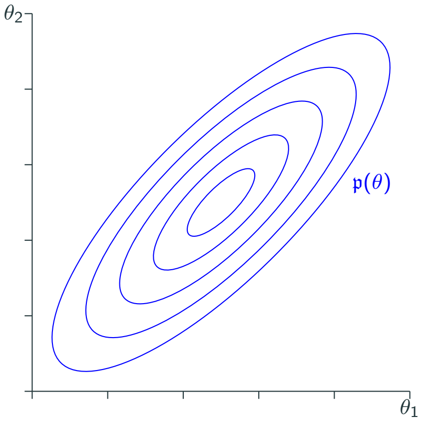
$$\underset{\mathfrak{q}\in\mathcal{Q}}{\operatorname{argmin}} \left(- \underset{\mathfrak{q}(\theta)}{\mathbb{E}}\left[\log \mathfrak{p}(\theta)\right] + \cancel{\underset{\mathfrak{q}(\theta)}{\mathbb{E}}\left[\log \mathfrak{q}(\theta)\right]} \right)?$$



KL divergence exercises

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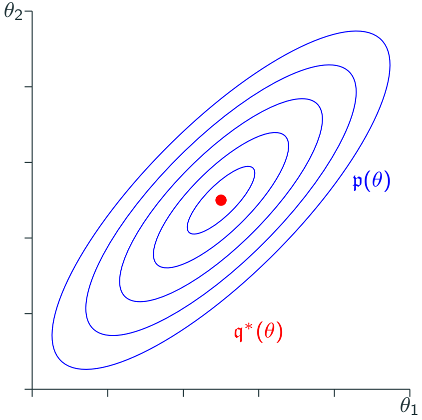

Without the entropy, the KL minimizer concentrates on the maximum of $\log \mathfrak{p}(\theta)$.

KL divergence exercises

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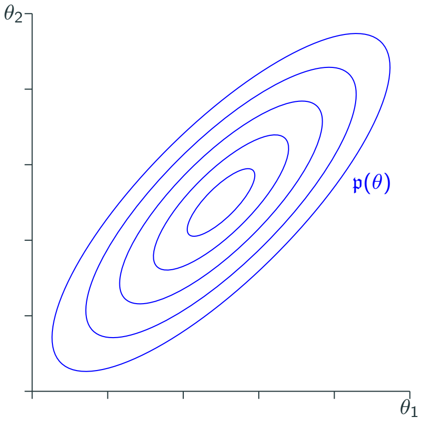

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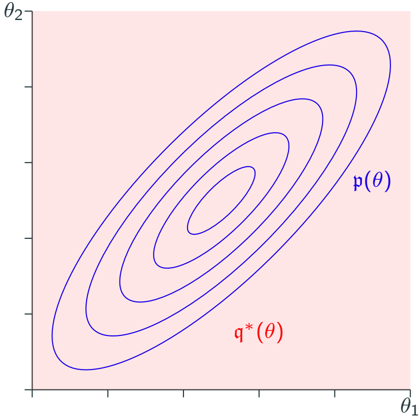


Without $\log \mathfrak{p}(\theta)$, the KL minimizer is infinitely dispersed.

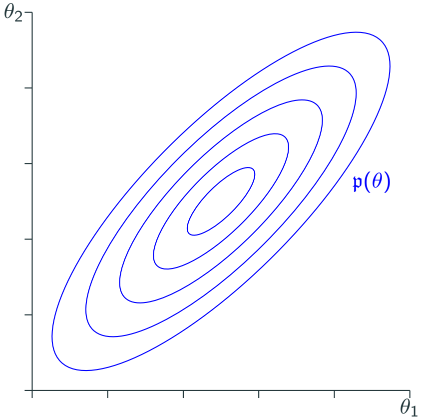
KL divergence exercises

$$\mathrm{KL}\left(\mathfrak{q}(\theta)||\mathfrak{p}(\theta)\right) = \\ -\underset{\mathfrak{q}(\theta)}{\mathbb{E}}\left[\log \mathfrak{p}(\theta)\right] + \underset{\mathfrak{q}(\theta)}{\mathbb{E}}\left[\log \mathfrak{q}(\theta)\right]$$

$\mathfrak{p}(\theta) = \text{Correlated bivariate normal}$

$\mathcal{Q} = \{\text{Point masses}\}$

What is $\mathfrak{q}^*(\theta) = \underset{\mathfrak{q}\in\mathcal{Q}}{\mathrm{argmin}}\, \mathrm{KL}\left(\mathfrak{q}(\theta)||\mathfrak{p}(\theta)\right)$?



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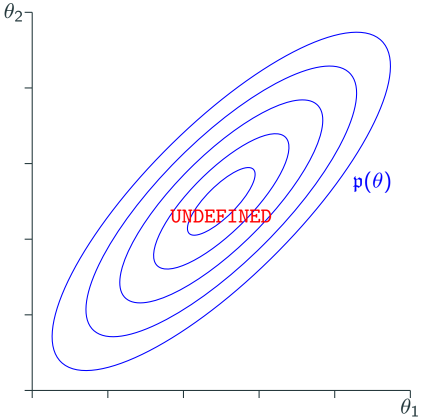


Without a common dominating measure, the KL divergence is undefined.

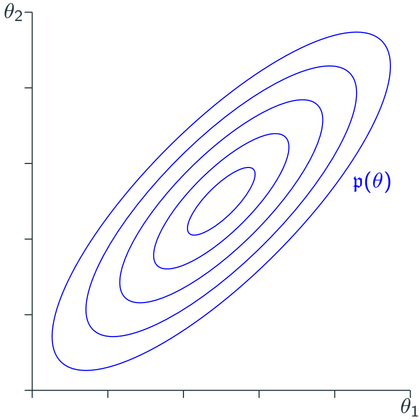
KL divergence exercises

$$\mathrm{KL}\left(\mathfrak{q}(\theta)||\mathfrak{p}(\theta)\right) = -\mathop{\mathbb{E}}_{\mathfrak{q}(\theta)}\left[\log \mathfrak{p}(\theta)\right] + \mathop{\mathbb{E}}_{\mathfrak{q}(\theta)}\left[\log \mathfrak{q}(\theta)\right]$$

$$\mathfrak{p}(\theta) = \text{Correlated bivariate normal}$$

$$\mathcal{Q} = \{\text{BVN with small, fixed variance}\}$$

What is $\mathfrak{q}^*(\theta) = \operatorname*{argmin}_{\mathfrak{q}\in\mathcal{Q}} \mathrm{KL}\left(\mathfrak{q}(\theta)||\mathfrak{p}(\theta)\right)$?



KL divergence exercises

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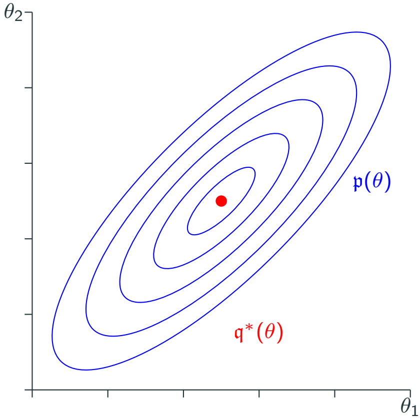

Sufficently concentrated distributions with constant entropy act like a point mass at the maximum of $\log \mathfrak{p}(\theta)$.

Recall the EM algorithm

$$\text{Observations: } y = (y_1, \dots, y_N)$$
$$\text{Unknown latent variables: } z = (z_1, \dots, z_N)$$
$$\text{Unknown global parameter: } \theta \in \mathbb{R}^D. \quad \text{We want: } \hat{\theta} = \underset{\theta}{\operatorname{argmax}} \log p(y|\theta).$$

The EM algorithm alternates between two steps. Starting at an iterate $\hat{\theta}_{(i)}$, repeat until convergence:

The E-step: Compute $Q_{(i)}(\theta) := \underset{p(z|y,\hat{\theta}_{(i)})}{\mathbb{E}} [\log p(y|\theta, z) + \log p(z|\theta)]$

The M-step: Compute the next iterate $\hat{\theta}_{(i+1)} := \underset{\theta}{\operatorname{argmax}} Q_{(i)}(\theta)$

The EM algorithm works / is useful when:

- The joint log probability $\log p(y|\theta, z) + \log p(z|\theta)$ is easy to write down
- The posterior $p(z|y, \theta)$ is easy to compute
- The marginalizing integral $p(y|\theta) = \int p(y|\theta, z)p(z|\theta)dz$ is hard

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Is the EM algorithm VI? **Can you spot the lie?**

The EM algorithm as VI

Let $\mathcal{Q}$ denote a family of distributions on z, parameterized by a finite-dimensional parameter η, such that $p(z|\theta, y) \in \mathcal{Q}$ for the observed y and all θ.

Let $\mathfrak{q}(z|\eta^*(\theta)) := p(z|\theta, y)$. Then:

$$
\begin{aligned}
\log p(y|\theta) &= \log p(y|\theta) + \mathrm{KL}\left(\mathfrak{q}(z|\eta^*(\theta))||p(z|\theta, y)\right) \\
&= \log p(y|\theta) + \underset{\eta}{\mathrm{argmax}}\left(-\mathrm{KL}\left(\mathfrak{q}(z|\eta)||p(z|\theta, y)\right)\right) & \bigstar \\
&= \underset{\eta}{\mathrm{argmax}}\left(\log p(y|\theta) - \mathrm{KL}\left(\mathfrak{q}(z|\eta)||p(z|\theta, y)\right)\right) \\
&= \underset{\eta}{\mathrm{argmax}}\left(\log p(y|\theta) + \underset{\mathfrak{q}(z|\eta)}{\mathbb{E}}\left[\log p(z|\theta, y) - \log \mathfrak{q}(z|\eta)\right]\right) \\
&= \underset{\eta}{\mathrm{argmax}}\left(\underset{\mathfrak{q}(z|\eta)}{\mathbb{E}}\left[\log p(y|\theta) \log p(z|\theta, y) - \log \mathfrak{q}(z|\eta)\right]\right) \\
&= \underset{\eta}{\mathrm{argmax}}\left(\underset{\mathfrak{q}(z|\eta)}{\mathbb{E}}\left[\log p(y, z|\theta)\right] + \underset{\mathfrak{q}(z|\eta)}{\mathbb{E}}\left[\log \mathfrak{q}(z|\eta)\right]\right) & \bigstar\bigstar
\end{aligned}
$$

The EM algorithm as VI

From the previous slide, the marginal MLE is given by

$$
\begin{aligned}
\hat{\theta} &:= \operatorname*{argmax}_{\theta} \log p(y|\theta) \\
&= \operatorname*{argmax}_{\theta} \operatorname*{argmax}_{\eta} \left(\log p(y|\theta) - \mathrm{KL}\left(\mathfrak{q}(z|\eta) || p(z|\theta, y)\right)\right) && \bigstar \\
&= \operatorname*{argmax}_{\theta} \operatorname*{argmax}_{\eta} \left(\mathop{\mathbb{E}}_{\mathfrak{q}(z|\eta)} \left[\log p(y, z|\theta)\right] + \mathop{\mathbb{E}}_{\mathfrak{q}(z|\eta)} \left[\log \mathfrak{q}(z|\eta)\right] \right) && \bigstar\bigstar
\end{aligned}
$$

Starting at an iterate $\hat{\theta}_{(i)}$:

The E-step:

1. For a fixed $\hat{\theta}_{(i)}$, optimize $\bigstar$ for η. Since only the KL divergence depends on η, the optimum is $\eta^*(\hat{\theta}_{(i)})$, and $\mathfrak{q}(z|\eta^*(\hat{\theta}_{(i)})) = p(z|\hat{\theta}_{(i)}, y)$.
2. Then use $\eta^*(\hat{\theta}_{(i)})$ to compute the expectation in $\bigstar\bigstar$ as a function of θ.

The M-step: Keeping η fixed at $\eta^*(\hat{\theta}_{(i)})$), optimize $\bigstar\bigstar$ as a function of θ to give $\hat{\theta}_{i+1}$. The entropy $\mathop{\mathbb{E}}_{\mathfrak{q}(z|\eta)} \left[\log \mathfrak{q}(z|\eta)\right]$ does not depend on θ and can be ignored.

$\Rightarrow$ The EM algorithm is coordinate ascent on $\log p(y|\theta) - \mathrm{KL}\left(\mathfrak{q}(z|\eta) || p(z|\theta, y)\right)$.

Corrolary: The EM algorithm converges to a local optimum of $\log p(y|\theta)$.

Conclusions

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